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Self-healing effects in the fabrication process of photonic crystals

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We demonstrate a self-healing effect of unwanted defects in the autocloning process: autocloning is a previously proposed technique to fabricate multidimensional periodic nanostructures by stacking up corrugated multilayers. With the self-healing effect, aperiodic perturbations in the initial periodic shape of the structure immediately disappear and the surface shape becomes periodic in a few cycles of stacking. If the perturbations exist in photonic crystal, they cause light-scattering loss and also make the boundaries between photonic bands and band gaps unclear. In other words, they make the attenuation of light at the frequency in photonic band gaps weak. Consequently, to attain uniformity of the shape automatically with this effect is very important in the fabrication process for practical photonic crystal devices. In this letter, we verify this phenomenon experimentally, and discuss the mechanism by comparison with process simulation. © *2000 American Institute of Physics.* [S0003-6951(00)01441-8]

Photonic crystals are multidimensional periodic structures having a high contrast of dielectric constants of materials. Since photons in the crystal are influenced by periodicity of the refractive index, photonic crystals have the following three main characteristics: photonic band gap,[1] optical anisotropy,[2] and high dispersion.[3,4] For applications in optical communication systems, various attractive devices utilizing either of these three characteristics have already been reported, for example, waveguides,[5] microcavities,[6] polarization splitters,[7] and superprisms.[3]

When photonic crystals are used in optical communication systems, their spatial periods must be less than 1 μm, making it very difficult to fabricate such multidimensional structures. Recently, several groups have reported successful fabrication of photonic crystals with full three-dimensional (3D) band gaps.[8,9] However, some breakthrough is still necessary to simplify the fabrication technique for industrial use.

We have already developed a simple reliable technique for fabricating photonic crystals, named ''autocloning,'' which is a technique of stacking films while preserving periodic surface corrugation, by a combination of sputter deposition and sputter etching. When we stack a-Si/SiO_2 alternate multilayers on a substrate with periodic grooves or holes as seeds for the corrugation, we can easily fabricate two-dimensional (2D) or 3D periodic structures having a high contrast, ~2.2, of dielectric constants,[10] as shown in Fig. 1.

Up to the present, we have demonstrated that the autocloned structures composed of Si/SiO_2 can be applied to optical communication systems.[3,7] Furthermore, we have recently succeeded in fabricating photonic crystals composed of TiO_2 and SiO_2 for visible wavelengths.[11]

In the autocloning processes, we have discovered that there are stationary states of surface shape when films are formed under appropriate conditions of sputter deposition and sputter etching. Moreover, we have experimentally verified the following characteristics of autocloning:

(1) Even though the initial shape is different from the stationary state, the shape immediately evolves into it [Fig. 2(a)] (Ref. 7).
(2) When there is a flat part larger than a period in the initial pattern, the part remains flat after dozens of layers are stacked [Fig. 2(b)] (Ref. 12).

In this letter, we report another effect of autocloning, the self-healing effect, which is a phenomenon in which aperiodic perturbations superposed on a periodic pattern are automatically eliminated, and in which the disordered shape is restored to the periodic uniform shape immediately. Due to this characteristic, we can automatically fabricate the uniform periodic structures and easily obtain the photonic crystals having high performance. We discuss a mechanism of the effect with an experimental demonstration and process simulation.

We stacked a-Si/SiO_2 multilayers and TiO_2/SiO_2 multilayers using bias-sputtering systems, which have two targets

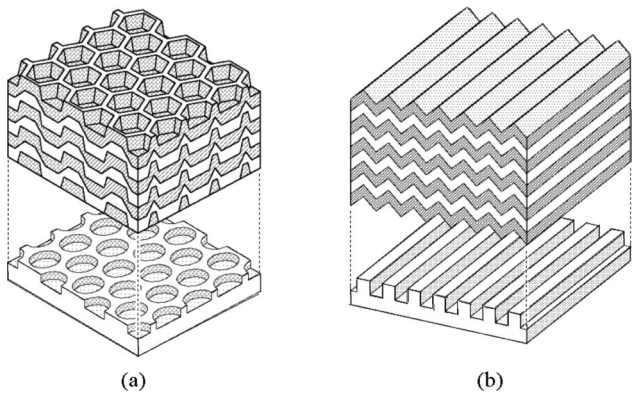

FIG. 1. Schematic figures of autocloned structures. (a) A 3D structure on a 2D patterned substrate. (b) A 2D structure on a one-dimensional (1D) patterned substrate.

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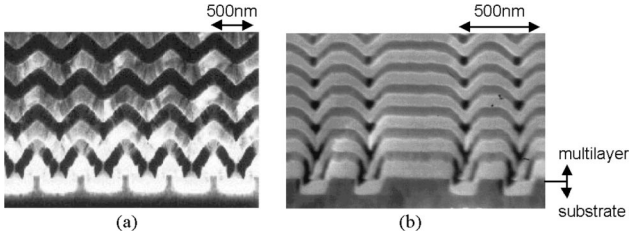

FIG. 2. Cross-sectional SEM photographs: (a) a-Si/SiO_2 multilayer stacked on a substrate whose shape is different from the stationary pattern. While several layers are stacked, the shape evolves into the stationary one. (b) a-Si/SiO_2 multilayer stacked on a substrate whose part is flat. Even after some layers are stacked, the part remains flat. The bright layers are a-Si, and the dark, SiO_2. SiO_2 is etched lightly by buffered HF to make the contrast clear.

in the vacuum chamber. Radio-frequency (rf) power can be fed to a substrate electrode and the two targets independently, hence, we can carry out sputter deposition and sputter etching simultaneously or sequentially. The fabrication process is as follows: we formed periodic grooves on Si wafers with SiO_2 (0.5 μm in thickness) using electron-beam (EB) lithography and reactive ion etching (RIE), then stacked the multilayers by the autocloning technique, that is, repeating sputter deposition and sputter etching alternately. After that, we cleaved the samples perpendicular to the grooves and observed the cleavages with scanning electron microscopy (SEM).

Figure 3(a) is a SEM photograph of a sample stacked on a substrate whose pattern is partially disordered. It shows that, after stacking a few layers, the disorder disappears and

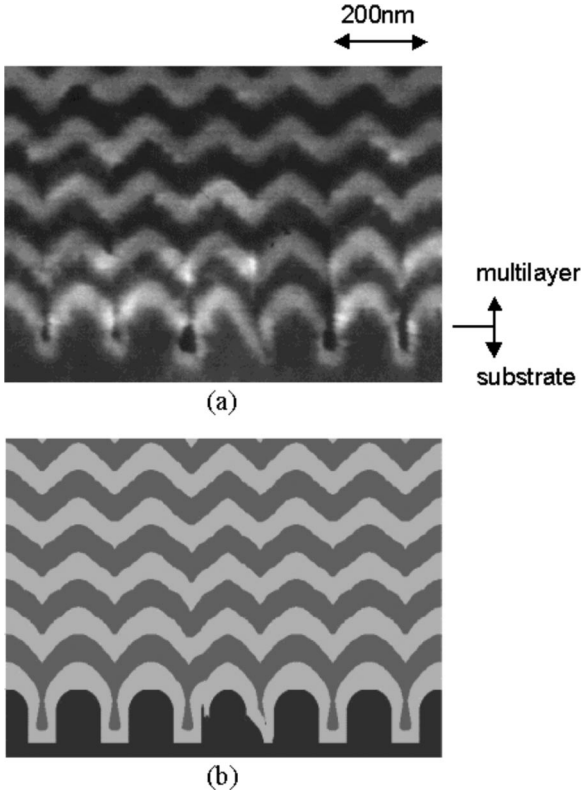

FIG. 3. (a) Cross-sectional SEM photograph of a stacked TiO_2/SiO_2 multilayer on a substrate whose pattern is partially disordered. The bright layer is TiO_2, and the dark, SiO_2. The irregular shape is restored immediately, and the shape becomes a homogeneous corrugation. (b) Simulation result of self-healing phenomenon by calculation.

FIG. 4. By the shadowing effect, ridges become wider and valleys become deeper (a). Next, by sputter etching at an angle-dependent etch rate, the preferred slope having the maximum sputter etching rate becomes dominant. By sputter-etched particles, redeposition occurs and valleys are filled in. When these phenomena balance each other out, the constant shape is preserved.

the shape becomes regular. The effect takes place in both cases of a-Si/SiO_2 and TiO_2/SiO_2 multilayers, ensuring that this effect is common to many material systems. This phenomenon is a self-healing effect, and the mechanism is discussed below.

In the autocloning processes, sputter deposition and sputter etching are carried out alternately, causing the following three phenomena on the film surface.[13]

(A) Deposition of sputtered particles coming from a target with a distribution of incident angles
(B) Sputter etching with an angular-dependent etching rate.
(C) Redeposition of film materials mainly generated by sputter etching.

By combining these three phenomena, the preservation of the corrugated shape is interpreted as follows. In the deposition process, by a shadowing effect caused by particles with a distribution of incident angles, ridges become wider and valleys become deeper [Fig. 4(a)]. After that, in the sputter etching process, the rounded ridges are sharpened because the slope at the angle with the maximum sputter etching rate is mainly formed. The bottoms of the valleys are simultaneously filled in by redeposition of particles sputtered from the film surface. As a result, a constant slope can be observed [Fig. 4(b)]. When these phenomena balance each other out, the surface shapes remain the same before and after a cycle of the processes, accordingly, the corrugated shapes are duplicated one after another.

We simulated the phenomenon demonstrated in Fig. 3(a) using a program in which the above three phenomena are expressed by formulas (NTT FANET Systems: PARADISEWORLD-2). We have already confirmed that one can simulate the preservation of the shape by using the program.[13] In the program, a film surface is represented by a group of small pixels. We can calculate the deposition/etching rate at each pixel of the surface.[14] In the case of the phenomenon A, the deposition rate can be calculated from the total amount of the particles coming to the pixel by considering a distribution of incident angles and a shadowing effect. In the case of phenomenon B, the etching velocity can be calculated from the angle of the surface where the pixel

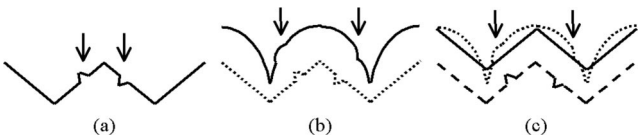

FIG. 5. Case of aperiodic perturbations on the surface (a). By deposition, the small pit is filled in and the small tip becomes dull (b). In the sputter etching process, the remaining convex and concave parts are shaped.

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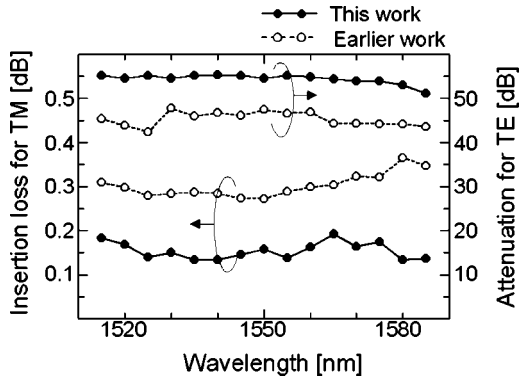

FIG. 6. Upper two lines and lower two lines express the attenuation for TE and the insertion loss for TM, respectively. Solid lines express the results of this work, and dashed lines express the earlier results (see Ref. 7).

lies to the incident direction of ions, normal to the substrate, and the angular dependence of the sputtering yield. In the case of C, the redeposition rate can be calculated assuming that redeposition particles come uniformly from the surrounding film surface to the pixel uniformly. Then we can obtain the surface evolution.

As shown in Fig. 3(b), the simulation result agrees well with the SEM photograph, indicating that the self-healing effect can be also interpreted by a combination of the above three phenomena. The mechanism of surface evolution can be described as follows.

As a simple model, we assume that there are smaller perturbations on the surface than the thickness of a layer [Fig. 5(a)]. When a layer is deposited, the small pit is filled in and the small tip becomes dull [Fig. 5(b)]. In the following process, the convex part is eroded away by sputter etching and a concave part is buried by redeposition. Consequently, the small perturbations immediately vanish, and smooth constant slopes can be obtained [Fig. 5(c)]. In other words, whether the shape is preserved or not depends on the ratio of the size of the perturbations to the amount of deposition and etching in a cycle.

Utilizing the self-healing effect, precisely periodic structures will be easily fabricated. For example, we discuss the performance of the proposed polarization splitter. The structure is shown in Fig. 1(b). When light is injected normal to the substrate, the light polarized perpendicular to the grooves is transmitted and the light polarized parallel to the grooves is reflected.[7] Figure 6 shows a graph of the insertion loss for TM polarization and the attenuation for TE polarization over a range of wavelengths. Owing to the self-healing effect, we can obtain smooth periodic interfaces between the *a*-Si layers and the SiO_2 layers in the autocloned structures, which can minimize light-scattering loss. The measured insertion loss is less than 0.2 dB with 10 periods at $\lambda = 1.55\,\mu$m. The origin of the improvement of the insertion loss as compared to the earlier work is twofold: The healing effect has previously decreased the scattering loss. We have also done investigation of reducing absorption. It has also contributed to the improvement. The residual loss is caused by absorption, and scattering loss is negligible. Moreover, if we stack a SiO_2 layer on the SiO_2 substrate by autocloning, we can fabricate the substrate with perfectly periodic grooves whose shapes are the same as the surfaces of the autocloned shape. Therefore, we can obtain high periodicity of the shape from the bottom of the multilayer to the top of the multilayers. It means that we can obtain high attenuation of light per period in the frequency range of band gaps. As a result, the measured attenuation is more than 50 dB with 10 periods at $\lambda = 1.55\,\mu$m. In the previous work when the SiO_2 layer was not stacked, it was about 45 dB with 10 periods.

In summary, we investigated the characteristics of autocloning against aperiodic perturbations by observing surface evolution from an intentional defect in the periodic patterned substrate. If the perturbations are not as large as the periodicity of the substrates, the shape is soon restored automatically after several layers of deposition, showing the self-healing effect. The key point of this phenomenon is the ratio between the size of the shape and the amount of deposition and etching in a cycle.

Owing to this unique characteristic, we can obtain perfectly uniform photonic crystals easily. For example, since perturbations in the shape of the substrate are inevitable in practical mass production, the self-healing effect is decisively important to achieve a high tolerance for fabrication errors of the substrates. Consequently, we conclude that the autocloning technique is suitable for industrialization.

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